**A variational approach to the Hamiltonian boundary value problem: existence and approximation**

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(joint work with Hartmut Schwetlick)

We consider the conservative dynamical system

$$\frac{d^2q(t)}{\mathrm{d}t^2} = -\nabla V(q) \ , \tag{1}$$

where $V$ is a smooth potential on $Q \subset \mathbb{R}^n$, and

$$q(0) = q_a \text{ and } q(T) = q_b \tag{2}$$

with $q_a, q_b \in Q$ and $T > 0$; we assume that the total energy $E$, defined as the sum of kinetic and potential energy, is fixed, so $T$ has to be determined.

A motivation for the analysis of this problem comes from Molecular Dynamics and other problems with complex energy landscapes. For example, $q_a$ and $q_b$ can be different conformational states of a molecule; then the Newtonian equations of motion (1) describe the vibrations of one conformation, followed by a rapid transition to the energetic well containing the other conformation, and vibrations in that well. This example illustrates two typical difficulties: the state space $Q$ can be high-dimensional (for example, $n \approx 400$ for relatively simple models of DNA motion); the timescale $T$ will be very long in comparison to the temporal scale of typical vibrations.

The problem of solving (1) with periodic boundary conditions has a long history, including existence results by Seifert [5], Weinstein [6], Rabinowitz [3].

The boundary value problem (1)–(2) is less studied. An existence result with additional differential-geometric assumptions on the underlying metric is due to Gordon [2].

We present an alternative existence result, where the *a priori* estimates depend on physical quantities, notably the total energy $E$ and the potential energy $V$. The method we employ resembles so-called string methods, but the particular setting we use allows us to prove the convergence of a suitable approximation.

The setting we use is that of Jacobi and Maupertuis; according to this classical principle, trajectories to (1) with total energy $E$ are suitably re-parametrised geodesics with respect to the *Jacobi metric*

$$g_{ij}(q) := 2(E - V(q))\delta_{ij}(q) \ ; \tag{3}$$

we recall that geodesics are critical points $\gamma$ of

$$L[\gamma] := \int_0^\tau \sqrt{g_{ij}(\gamma(s))\dot\gamma^i(s)\dot\gamma^j(s)}\,\mathrm{d}s \ , \tag{4}$$

where $q = q(s)$, $q(0) = q_a$, $q(\tau) = q_b$. For Jacobi's metric, this is

$$L[\gamma] := \int_0^\tau \sqrt{2(E - V(q))\,\langle \dot q, \dot q\rangle}\,\mathrm{d}s \ . \tag{5}$$

Physical time can then be recovered via the explicit formula

$$t = \int_0^\tau \sqrt{\frac{\langle \dot{q}, \dot{q} \rangle}{2(E-V)}} \, \mathrm{d}s \ . \tag{6}$$

The advantage of the variational method (5) is its elliptic nature; the existence of periodic solution is thus often studied in this setting [5, 6]. An argument going back to Birkhoff [1] can in this case provide a constructive existence proof.

We provide a similar result for the boundary value problem, but with a different focus: Given $q_a$ and $q_b$, bounds can be given on the choice for $E$ such that the existence of a trajectory can be guaranteed. The argument uses discrete curvature bounds to obtain a neighbourhood of $q_a$ and $q_b$ which is invariant under a flow.

While in principle such an argument is not hard once a curvature bound yielding an invariant region is found, we choose to complicate the proof so that it yields in the end a constructive convergent approximation by line segments. Line segments are Euclidean geodesics, so it is natural to use piecewise constant approximations of the Jacobi metric (3). The computation of the length is then in principle simple. However, care has to be taken of the scaling. It can be shown that locking and other artificial effects can be avoided if three different scales are considered: one for the discretisation width $\epsilon_0$ of polygonal approximations for $\gamma$, a finer one for the step width of the Birkhoff step and an even finer one for the computation of the length.

Unlike the continuous (original) Birkhoff step, the argument requires a grid refinement, even a sequence of refinements $\epsilon_k := 2^{-k}\epsilon_0$ (and suitable refinements of the two other scales involved). It can then be shown that the Birkhoff procedure stops on every discrete level $k$ after finitely many steps, yielding a limit polygon $\gamma_k$. It can be shown that $\gamma_k \to \gamma \in C^{1,1}$ as $k \to \infty$, where $\gamma$ is a geodesic graph.

We close by remarking that, rather than relying on a Birkhoff procedure, a parabolic flow with an artificial time can be used as a steepest descent procedure to the elliptic limit associated with (5). A numerical implementation shows that this is an efficient string method [4]; a theoretical underpinning of this flow in form of a convergence proof is however missing.

The homogenisation of this problem (that is, the computation of effective Hamiltonians for potentials $V_\epsilon$ with wiggly contributions in the limit $\epsilon \to 0$) was also mentioned as open problem in the discussion at the meeting. Also, the result presented here is deterministic. Extensions to a stochastic setting (e.g., within the Freidlin-Wentzell theory or for thermostats) are presently not available.

## References


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